

Wick's theorem for matrix product states

R. Hübener¹, A. Mari^{1,2,3}, and J. Eisert¹

¹ *Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Berlin, Germany*

² *Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany and*

³ *NEST, Scuola Normale Superiore and Istituto di Nanoscienze - CNR, Pisa, Italy*

Matrix product states and their continuous analogues are variational classes of states that capture quantum many-body systems or quantum fields with low entanglement; they are at the basis of the density-matrix renormalization group method and continuous variants thereof. In this work we show that, generically, N -point functions of arbitrary operators in discrete and continuous translationally invariant matrix product states are completely characterized by the corresponding two- and three-point functions. Aside from having important consequences for the structure of correlations in quantum states with low entanglement, this result provides a new way of reconstructing unknown states from correlation measurements *e.g.* for one-dimensional continuous systems of cold atoms. We argue that such a relation of correlation functions may help in devising perturbative approaches to interacting theories.

I. INTRODUCTION

Quantum states of many-body systems or fields are characterized by their N -point correlation functions. Unsurprisingly, given their central status in the respective theories, there are many ways in which such correlation functions can be book-kept in terms of as simple as possible mathematical objects. For instance, prominent perturbative methods for the description of interacting field theories make extensive use of the relation between high order and two-point correlators [1–4]. These methods, supported by ‘Wick’s’ or Wick’s Theorem [3, 4] (depending on context), give rise to a practical way of identifying the propagators as the basic objects for the description of the situation at hand, as well as an interpretation in terms of virtual processes.

In this work we show that, remarkably, generic translationally invariant matrix product states [5–8] and their continuous analogues, cMPS or holographic states [9–11] are completely characterized by their two- and three-point functions. These states comprise a variational state class that approximates states with limited spatial entanglement well—a ubiquitous property for good reasons [7, 8]—and are at the basis of the seminal density-matrix renormalization group (DMRG) method [8] and continuous versions thereof [9, 10]. What is more, in our approach states and corresponding operators can be constructed such that their N -point correlation functions are completely characterized by their correlators of up to arbitrary odd order. We do so by proposing an explicit construction procedure of how to reconstruct higher-order correlation functions from lower order ones. This insight has a number of interesting consequences.

To start with, a fruitful research program has emerged in recent years of revisiting questions in many-body theory within the variational set of matrix product states, now seen as a “theoretical laboratory”. This approach has the very appealing feature that some links and statements that are in all generality too hard to capture analytically can be formulated in a completely rigorous fashion. In this mindset, complete classifications of quantum phases have been given [12], new instances of Lieb-Schultz-Mattis theorems proven [13], or phase transitions of arbitrary order identified [14]. Our statement provides a new tool to grasp the structure of matrix product states and their analogues for quantum fields.

Our result also identifies matrix product states as a variational class that is similar to, but yet beyond, quasi-free approaches. This observation may be even more interesting in the light of the fact that it is not straightforward to construct natural classes generalizing Gaussian states: For example, it is known that any unitary evolution generated by quadratic polynomials in the canonical coordinates maps Gaussian states to Gaussian states. If one looks at

the closure of the unitaries generated by the quadratic polynomials and a single further term, say, of third order, one does not arrive at a meaningful new variational class, but in fact generates all unitaries [15].

More practically speaking, our result clearly opens up novel ways to think of reconstruction methods for quantum states. Most prominently in this direction, it seems unclear how to obtain precise knowledge about the quantum states of continuous systems such as cold atoms on top of atom chips [16] from correlation measurements—let alone complete tomographic knowledge. Such information would, however, be most valuable to analyze the experiments made with such systems in and out of equilibrium. The present result shows how continuous-matrix product states can be reconstructed from low order correlation functions only *e.g.* obtained from atom detectors [17], with a phase reference obtained by interference.

Finally, the most important implications may come from the description of the fundamental insight into the structure of correlations as such. In a way, our result shows that states of limited entanglement have interesting inherent structural properties, comparable to the structural properties of meromorphic functions.

II. SETTING

The main theorem of this paper applies to *generic* translationally invariant (continuous) matrix product states in the thermodynamic limit. Let us define what this means and fix some basic notation.

A. Matrix product states

A discrete matrix product state vector of an N -partite spin system with periodic boundary conditions is given by

$$|\psi_{\text{MPS}}\rangle = \sum_{s_N, \dots, s_1} \text{Tr} \left[A^{(N)}[s_N] \dots A^{(1)}[s_1] \right] |s_N, \dots, s_1\rangle, \quad (1)$$

where the $A^{(i)}[s_i] \in \mathbb{C}^{d \times d}$ are finite dimensional complex matrices. In this work we will focus on the thermodynamic limit, *i.e.* $N \rightarrow \infty$, and the translationally invariant case, *i.e.* $A^{(i)}[s] = A^{(j)}[s]$ for all i, j . The finite bond dimension d will be arbitrary but fixed. In this setting, correlation functions of a set of operators $\{O_j\}$ labeled by an index j and with support on (different) sites

i_k with $0 = i_1 < \dots < i_N$ take the form

$$\langle O_{j_N}^{(i_N)} O_{j_{N-1}}^{(i_{N-1})} \dots O_{j_1}^{(i_1)} \rangle = \text{Tr} \left[M^{[j_N]} E^{i_N - i_{N-1} - 1} M^{[j_{N-1}]} \dots M^{[j_1]} E^\infty \right] =: C_{\mathbf{j}}^{(3)}(\mathbf{n}), \quad (2)$$

with $M^{[j]} = \sum_{m,n} A^*[m] \otimes A[n] \langle m | O_j | n \rangle$, and the transfer matrix $E = \sum_s A^*[s] \otimes A[s]$. The star indicates complex conjugation of the matrix elements. We have written the distances in a compact form as $\mathbf{n} = (i_2 - i_1 - 1, \dots, i_N - i_{N-1} - 1) \in \mathbb{Z}^{N-1}$ and summarized likewise $\mathbf{j} = (j_1, \dots, j_N)$. It is possible to consider finite dimensional and infinite dimensional local systems; in the latter case the matrices $A[s]$ have to be chosen such that the infinite sums converge.

The expectation values are invariant under simultaneous conjugation of all $M^{[j]}$ and E with some invertible matrix, making it possible to consider an equivalent formulation where E is in its Jordan normal form (JNF), i.e. $E \mapsto J(E)$. We call the MPS *generic* if $J(E)$ has non-degenerate diagonal entries μ_1, \dots, μ_{d^2} and, moreover, if the largest absolute value occurs only once. We order the diagonal elements by their absolute value, in descending order. Note that in the thermodynamic limit normalization implies $|\mu_i| \leq 1$, where the one with the largest magnitude equals unity, i.e. $\mu_1 = 1$. In the future, we will simply say eigenvectors when we mean the *right* eigenvectors, i.e. $E|i\rangle = \mu_i|i\rangle$. The number of Schmidt coefficients, and hence the entanglement belonging to any contiguous bipartition of regions is limited by $2d$.

B. Continuous MPS

A one dimensional non-relativistic bosonic quantum field can be described in terms of field operators $\Psi(x)$ and $\Psi^\dagger(x)$, with $[\Psi(x), \Psi(x')^\dagger] = \delta(x - x')$ and $\Psi(x)|0\rangle = 0$, where $|0\rangle$ is the vacuum. A particular class of one dimensional quantum fields is that of continuous MPS (cMPS) or holographic states [9, 10],

$$|\psi_{\text{cMPS}}\rangle = \text{Tr}_{\text{aux}} \left[\mathcal{P} e^{\int_0^L dx Q(x) \otimes \mathbb{1} + R(x) \otimes \Psi^\dagger(x)} \right] |\Omega\rangle, \quad (3)$$

where $Q(x)$ and $R(x)$ are x -dependent finite-dimensional complex matrices acting in a d -dimensional auxiliary space. Similar to the case of MPS, we focus on translationally invariant cMPS, having constant Q and R , in the thermodynamic limit $L \rightarrow \infty$. It is useful to introduce the Liouvillian (see appendix) matrix defined as

$$T = Q^* \otimes \mathbb{1} + \mathbb{1} \otimes Q + R^* \otimes R. \quad (4)$$

A state of such a quantum field is completely characterized by all the possible normal ordered correlation functions of the operators $\Psi(x)$ and $\Psi^\dagger(x)$ e.g.

$$\langle \Psi^\dagger(x_2) \Psi^\dagger(x_5) \dots \Psi(x_4) \Psi(x_3) \Psi(0) \rangle. \quad (5)$$

where the order of position labels is such that they increase in size from left to right within the Ψ^\dagger , decrease within the Ψ , and $0 = x_1 < \dots < x_N$. Correlation functions of cMPS are given by expressions involving only the auxiliary space. Let e^{T^∞} be a short notation for $\lim_{L \rightarrow \infty} e^{TL}$. In the example of a 2-point function, we have

$$\langle \Psi^\dagger(x) \Psi(0) \rangle = \text{Tr} \left[(\mathbb{1} \otimes R) e^{Tx} (R^* \otimes \mathbb{1}) e^{T^\infty} \right], \quad (6)$$

according to the well-known expressions for expectation values in cMPS. Sometimes we might have access to the density only, i.e. to the operator $\Psi^\dagger(x) \Psi(x)$, whose correlations are [9, 10], for instance,

$$\langle \Psi^\dagger(0) \Psi^\dagger(x) \Psi(x) \Psi(0) \rangle = \text{Tr} \left[(R^* \otimes R) e^{Tx} (R^* \otimes R) e^{T^\infty} \right]. \quad (7)$$

Let us go back to Eq. (5). For translationally invariant cMPS, we consider the differences between points, $\tau_i = x_{i+1} - x_i$ and summarize them in a vector notation $\boldsymbol{\tau} = (\tau_1, \tau_2, \dots, \tau_{N-1}) \in \mathbb{R}^{N-1}$. Let the matrices $M^{[j]}$ be equal to $R^* \otimes \mathbb{1}$, $\mathbb{1} \otimes R$ or $R^* \otimes R$ etc. With this notation we represent all N -th order correlation functions in a compact and straightforward way. For example

$$\langle \Psi^\dagger(x_2) \Psi^\dagger(x_3) \Psi(x_2) \Psi(0) \rangle = \text{Tr} \left[M^{[1]} e^{T\tau_2} M^{[3]} e^{T\tau_1} M^{[2]} e^{T^\infty} \right] =: C_{\mathbf{j}}^{(3)}(\boldsymbol{\tau}) \quad (8)$$

with $\boldsymbol{\tau} = (x_2, x_3 - x_2)$, $\mathbf{j} = (1, 3, 2)$, and $M^{[1]} = R^* \otimes \mathbb{1}$, $M^{[2]} = \mathbb{1} \otimes R$ and $M^{[3]} = R^* \otimes R$. Note that also in this case a gauge transformation is possible, corresponding to a simultaneous conjugation of T and the matrices $M^{[j]}$ by an invertible matrix, so that we can always go to a picture where T is in its JNF. The relationship between cMPS and channels directly implies [18] that the diagonal elements $\lambda_1, \lambda_2, \dots, \lambda_{d^2}$ of $J(T)$ are closed under conjugation. We call the cMPS *generic* if $J(T)$ has a non-degenerate diagonal and, moreover, the largest real part occurs only once. We order the eigenvalues in descending order by their real parts; the normalization of cMPS implies that it is non-positive and the largest one is zero, i.e. even $\lambda_1 = 0$. Similar to MPS, cMPS have limited bipartite entanglement between contiguous regions: the number of Schmidt coefficients is limited by $2d$. As in the case of MPS, we will simply say eigenvectors when we mean the *right* eigenvectors, i.e. $e^T|i\rangle = e^{\lambda_i}|i\rangle$.

III. MAIN RESULT

In general, to characterize the full state of a quantum system one needs to specify all the correlation functions. One may ask the following question: “*Is it possible to completely characterize a (continuous) matrix product state from low order correlation functions?*” With the only initial assumption of a given bond dimension d , in this work we will show how to:

1. Certify that the given (continuous) MPS is generic.
2. Reconstruct the full state of a (continuous) MPS from low order correlation functions once the previous property has been verified.

In order to accomplish the first task we need to test if the diagonals of $J(E)$, $J(T)$ are non-degenerate (see the corresponding sections). The diagonal elements will appear as poles of the Z-respectively Laplace-transform of the correlation functions. The second task is more involved since it requires a careful analysis of the structure of correlation functions, instead of the mere knowledge of the diagonal. Both aspects will be studied in detail in the following.

A. Data structure and transformations

We will use both the Z- and the Laplace transform of correlation functions in their multi-dimensional form. For discrete MPS, the

Z-transform is applicable

$$\mathcal{Z}_{\mathbf{j}}^{(N)}(\mathbf{s}) = \sum_{n_1, \dots, n_N} s_1^{n_1} \dots s_N^{n_N} C_{\mathbf{j}}^{(N)}(\mathbf{n}), \quad s_1, \dots, s_N \in \mathbb{C}. \quad (9)$$

Similarly, we have a Laplace transformation of the cMPS correlation functions

$$\mathcal{L}_{\mathbf{j}}^{(N)}(\mathbf{s}) = \int_0^\infty d^{N-1} \tau e^{-\mathbf{s} \cdot \boldsymbol{\tau}} C_{\mathbf{j}}^{(N)}(\boldsymbol{\tau}), \quad s_1, \dots, s_N \in \mathbb{C}. \quad (10)$$

Depending on the correlation data, these transformations will not converge everywhere. The key observation is the following. A close inspection of the correlation functions reveals that under the assumption of a non-degenerate diagonal of $J(E)$, we have

$$C_{\mathbf{j}}^{(N)}(\mathbf{n}) = \sum_{k_1, \dots, k_{N-1}=1}^{d^2} c_{\mathbf{j}}^{(N)}(k_1, \dots, k_{N-1}) \times (\mu_{k_{N-1}})^{n_{N-1}} \dots (\mu_{k_1})^{n_1}, \quad (11)$$

where

$$c_{\mathbf{j}}^{(N)}(k_1, \dots, k_{N-1}) = \langle 1 | M^{[j_{N-1}]} | k_{N-1} \rangle \langle k_{N-1} | M^{[j_{N-2}]} \dots | k_1 \rangle \langle k_1 | M^{[j_1]} | 1 \rangle, \quad (12)$$

and $\{|k\rangle\}$ denotes the basis where E obtains JNF. Note that in this basis $E^\infty = |1\rangle\langle 1|$. Considering that $|\mu_i| \leq 1$ with $\mu_1 = 1$, we deduce that the Z-transform—as a function in the complex variables $\{s_1, \dots, s_{N-1}\}$ —converges within the product of unit disks around the origin, yielding a meromorphic function. It is possible, starting from this region, to reconstruct the whole function (its poles and the residues) by analytic continuation. Another way of dealing with *e.g.* experimental data, would be to fit functions of the given form using only the unit disk as support. For partial reconstruction of experimental data, see also Sec. IV D, where it is shown that poles corresponding to long-range behavior are close to the unit circle. Summarizing, we have access to

$$\mathcal{Z}_{\mathbf{j}}^{(N)}(\mathbf{s}) = \sum_{k_1, \dots, k_{N-1}}^{d^2} \frac{c_{\mathbf{j}}^{(N)}(k_1, \dots, k_{N-1})}{(1 - \mu_{k_1} s_1) \dots (1 - \mu_{k_{N-1}} s_{N-1})}. \quad (13)$$

Similar considerations apply to cMPS correlations, which, under the assumption of non-degenerate $J(T)$, can be expressed as

$$C_{\mathbf{j}}^{(N)}(\boldsymbol{\tau}) = \sum_{k_1, \dots, k_{N-1}=1}^{d^2} c_{\mathbf{j}}^{(N)}(k_1, \dots, k_{N-1}) \times e^{\lambda_{k_1} \tau_1} \dots e^{\lambda_{k_{N-1}} \tau_{N-1}} \quad (14)$$

with the same symbols $c_{\mathbf{j}}^{(N)}(k_1, \dots, k_{N-1})$ as defined in Eq. (12). The integral in Eq. (10) yields meromorphic functions in higher dimensions of the form

$$\mathcal{L}_{\mathbf{j}}^{(N)}(\mathbf{s}) = \sum_{k_1, \dots, k_{N-1}}^{d^2} \frac{c_{\mathbf{j}}^{(N)}(k_1, \dots, k_{N-1})}{(\lambda_{k_1} - s_1) \dots (\lambda_{k_{N-1}} - s_{N-1})}. \quad (15)$$

According to $\Re \lambda_i \leq 0$, the region of convergence of the integral in Eq. (10) is the product of complex half-planes with positive real part. As a meromorphic function, it can be reconstructed using this data. Note that now $e^{T^\infty} = |1\rangle\langle 1|$ and poles reflecting long-range behavior now lie close to the imaginary axis.

The fact that the diagonal of $J(E)$ and $J(T)$ is non-degenerate and has only finitely many elements played a crucial role in the derivation of the form of Eq. (11) and (14). This procedure is stable under the influence of noise in the sense that the residues of the poles and their positions are continuous in the matrix entries. For the purposes of the present work, we will postpone questions of the scaling of the computational effort of the classical post-processing in the precision of the input as well as in the bond dimension of the MPS and cMPS [19] and focus on the possibility of reconstruction of higher correlation functions from lower ones as such.

B. Reconstruction theorem

The form of the Eqs. (13) and (15) implies that all poles are elements of $\{\lambda_i\}$ and $\{\mu_i^{-1}\}$, respectively. Depending on whether the corresponding residues $c_{\mathbf{j}}^{(N)}(k_1, \dots, k_{N-1})$ are zero or not, the transforms of the correlation data may or may not reveal poles at these points. This makes it useful to give the following definition

Definition 1 (*p*-number) *Given a (continuous) MPS with bond dimension d , we define the p -number as the minimum order p such that d^2 distinct poles appear in the Z- or Laplace transforms, respectively, in at least one correlation function of order less or equal to p . If the minimum does not exist we say that the p -number is infinite.*

Note that in this definition, we only need *one* correlation function of *any* subset of operators of interest to show all poles, in order to derive the p -number. This provides a solution to the first task: If the p -number of a (continuous) MPS is finite, we can directly claim that E or T have a non-degenerate Jordan diagonal.

Now we are going to study in more detail not only the poles but the full structure of correlation functions of (continuous) MPS. We work in the basis where E or T are in JNF. If a function $\mathcal{Z}_{\mathbf{j}}^{(N)}$ or $\mathcal{L}_{\mathbf{j}}^{(N)}$ is given, each coefficient $c_{\mathbf{j}}^{(N)}(k_1, \dots, k_{N-1})$ can be extracted by finding the residue of the corresponding multi-pole. We can finally state the main theorem:

Theorem 1 (Computing higher from lower correlation functions)

A generic, translationally invariant (continuous) MPS in the thermodynamic limit with p -number p is completely characterized by the correlation functions of order $\ell \leq 2p - 1$.

Proof: We merely need to consider the case in which p is finite. From the definition of the p -number we know that $J(E)$, respectively $J(T)$, have a non-degenerate diagonal in the JNF, whose entries can be recovered from (the pole structure of the transforms of) the correlation functions of order $\ell' \leq p$. This reduces the reconstruction of correlation functions to the reconstruction of the coefficients in Eq. (12). The problem is now to express every coefficient

$$c_{\mathbf{j}}^{(N)}(k_1, \dots, k_{N-1}) = M_{1, k_{N-1}}^{[j_{N-1}]} M_{k_{N-1}, k_{N-2}}^{[j_{N-2}]} \dots M_{k_1, 1}^{[j_1]}, \quad (16)$$

each associated with a unique set of poles, in terms of low order coefficients $c^{(\ell)}$ with $\ell \leq 2p - 1$. From the definition of the p -number we know that for each index k there is at least one non-zero coefficient $c_{\mathbf{j}(k)}^{(p(k))}(\dots, k, \dots) \neq 0$, with $p(k) \leq p$ and fixed $\mathbf{j}(k)$, having k as one of its indices. This allows us to write d^2

different versions of the identity (this is a scalar)

$$1^{(k)} = \frac{M_{1,\star}^{[j(k)_{p(k)-1}]} \dots M_{\star,k}^{[j(k)_{\ell'}]} M_{k,\star}^{[j(k)_{\ell'-1}]} \dots M_{\star,1}^{[j(k)_1]}}{c_{\mathbf{j}(k)}^{(p(k))}(\dots, k, \dots)}, \quad (17)$$

where $k = 1, 2, \dots, d^2$, and the symbol \star stands for other indices which are irrelevant. Now we reorder the matrix elements in the numerator by shifting all matrix elements on the r.h.s. of the index k simultaneously to the l.h.s., leaving the order of the other indices untouched, *i.e.* in the following way

$$1^{(k)} = \frac{M_{k,\star}^{[j(k)_{\ell'-1}]} \dots M_{\star,1}^{[j(k)_1]} M_{1,\star}^{[j(k)_{p(k)-1}]} \dots M_{\star,k}^{[j(k)_{\ell'}]}}{c_{\mathbf{j}(k)}^{(p(k))}(\dots, k, \dots)}. \quad (18)$$

We can finally put all these resolutions of the identity between the matrix elements in Eq. (16)

$$c_{\mathbf{j}}^{(N)}(k_1, \dots, k_{N-1}) = M_{1,k_{N-1}}^{[j_{N-1}]} 1^{(k_{N-1})} M_{k_{N-1},k_{N-2}}^{[j_{N-2}]} 1^{(k_{N-2})} \dots 1^{(k_1)} M_{k_1,1}^{[j_1]}. \quad (19)$$

We recognize, in the numerator, several new strings of matrix elements resulting from the insertion. They have the same structure as in Eq. (16) but a lower order $\ell \leq 2p - 1$. This means that, for every N , all the coefficients $c_{\mathbf{j}}^{(N)}$ can be written in terms of $c_{\mathbf{j}}^{(\ell)}$ with $\ell \leq 2p - 1$. In other words, correlation functions of order less or equal to $2p - 1$ are enough to reconstruct all the others. This proves the validity of the theorem. \square

IV. DISCUSSION

A. Example

It is instructive to consider the following case. Given an MPS or a cMPS with finite d , let the operators O_j and the state be such that the corresponding matrices $\tilde{M}^{[j]} = X M^{[j]} X^{-1}$ have only *non-zero* elements. Here $J(\cdot) = X \cdot X^{-1}$ is the conjugation that takes E, T to their JNF. Note that the probability to have this situation in an experiment, or using a randomized (continuous) MPS and operators O_j , is one. Under this condition, all two-point function transforms show all the poles, hence $p = 1$. Computationally, all residues of all the poles of all N -point functions with $N \leq 3$ can be obtained. Hence we can, using the construction above, give explicit formulas that express all N -point functions in terms of the 2- and 3-point functions. See also Section IV B.

B. Applications in tomography

The framework established here opens up ways to reconstruct unknown states from correlation data alone, in the sense of tomographic reconstruction. Such tomographic reconstructions based on data sets such as MPS and cMPS are important not only because MPS (and cMPS) form such a ubiquitous and important class of quantum states, as the states that capture situations of low entanglement well. For scalable reconstructions of states of quantum many-body systems, one necessarily has to make use of data structures that are efficient in the system size. In this way, the approach proposed here gives rise to a complementary picture of viewing tomography of MPS to the method of Ref.

[21], where the reconstruction is based on tomographic estimation of certain reduced states. The ideas presented here seem more promising, however, for the tomographic reconstruction of quantum field states and continuous systems, for which no method is known altogether. Notably, from correlation data of atoms counting experiments [16, 17] with or without a phase reference, a construction of quantum field states can be done along the above lines [22].

The aim of a reconstruction is to give (a representation of) a positive functional on (a representation of) operators corresponding to our measurements that generates the given data. This functional itself will be given by formulas 2 and 8, respectively, hence the quantities to be derived from the data are matrices $J(E)$, $J(T)$ and $M^{[j]}$ s. Because the origin of the formulas of our reconstruction is a (continuous) MPS ansatz—modified by some gauges only—we are already certain of the positivity of such formulas. We consider two more aspects.

First, any reconstruction procedure can at best find a representative of the equivalence class of all (continuous) matrix product states that are identical up to a gauge transformation. From Eqs. (2) and (8), we immediately derive that simultaneous conjugations of the transfer matrix E and the operator matrices $M^{[j]}$ —analogously the Liouvillian T and $M^{[j]}$ —by an invertible matrix leaves the expectation values invariant. So does the transformation $Q \mapsto Q + \alpha \mathbb{1}$, which changes the norm of the cMPS. These are gauge transformations and do not change the observable physics. Some of these transformations have been performed to obtain the pole structure in the explicit form, diagonalizing the E and T and ordering the diagonal elements. Hence we have “fixed the gauge”, but only partially.

Second, we need a promise of the dimensionality d of the matrices. The p -number then tells us if the experimental data is consistent with this promise and if we “see enough structure in the data”, *i.e.* if we can use it for a full reconstruction of one representative. As we have seen in Section (IV A) in all cases except a set of measure zero, the matrices $M^{[j]}$ contain no zeros as elements and the p -number is one. This allows for a reconstruction along the following lines. Let us assume for simplicity to have only one operator M . The case of more $M^{[j]}$ is then straightforward.

After the observed data has been processed, we have obtained the values of the variables occurring in Eqs. (11) (or Eq. (14)). We only need the two- and three-point functions. In particular, we found the position of the poles $\{\mu_i^{-1}\}$ (or $\{\lambda_i\}$) of the transforms of the correlators. The diagonal elements of the matrix $J(E)$ (or $J(T)$) are in one-to-one correspondence to the poles of the two-point function when $p = 1$. We also found the residues $c_{\mathbf{j}}^{(N)}(k_1, \dots, k_{N-1})$, for $N = 2, 3$, which determine the operator matrices M . We now need to reconstruct M and we are done.

If one uses a scalar $a_k \neq 0$

$$M_{k,1} \mapsto a_k M_{k,1}, \quad M_{1,k} \mapsto a_k^{-1} M_{1,k} \quad (20)$$

then the M s change, but the two- and three-point functions (and the pole structure) do not. This gauge comes from the conjugation of E (or T) and the M s with an invertible diagonal matrix and has not been fixed before. We use this freedom to set $M_{1,k} = 1$. Accordingly, we obtain, via Eq. (19), directly from the residues of the poles

$$M_{k,1} = c^{(2)}(k). \quad (21)$$

The remaining elements of M are obtained from Eq. (19) via

$$M_{k,\ell} = c^{(3)}(k, \ell) / c^{(2)}(\ell). \quad (22)$$

This is enough for the reconstruction. If we have more data (*e.g.* higher N -point functions), it can be used as a consistency criterion for the assumptions. If the data is noisy, the formulas will not be consistent, but maximum-likelihood estimations can be performed and can profit from more data and the relations discussed in this article [22].

C. Arbitrary odd order dependence

To construct (continuous) MPS together with a set of operators that is dependent on correlators up to an arbitrary odd order, instead of two- and three-point functions, one has to solve for the equations given in Eq. (12). The aim is to choose $J(E)$, respectively $J(T)$, and the operators $\{O_j\}$ such that they do *not* fulfill the p -number condition up to a desired order p . Essentially, the corresponding matrices $\{M^{[j]}\}$ have to be sparse enough. As the matrix dimension d is to be chosen freely, this requirement can be met in a construction.

D. Judging the importance of poles and the treatment of infinite dimensional auxiliary space

The decay behavior of contributions to the correlations follows directly a) in the case of MPS from the absolute value of the corresponding poles, and b) in the case of the cMPS from their real part. (Note the relation between poles and diagonal elements: $s_i = \mu_i^{-1}$ and $s_i = \lambda_i$, respectively.) Hence their position on the complex plane is decisive. This means that the MPS poles describing slow decay are situated close to the unit circle, and the cMPS poles of this kind are close to the imaginary axis.

As interesting states of most physical models in 1D have an infinite Schmidt number even if they obey an area law and have quickly decaying Schmidt coefficients [7], the order of the poles corresponding to their decay behavior is important when reconstructing only a subspace of the auxiliary space. According to the consideration above, it is hence feasible to compute only relevant MPS matrix dimensions from a given set of experimental correlation data, retaining *e.g.* only long-range behavior in the description.

V. OUTLOOK

A stimulating insight is given by the mathematical structure of the correlations, which are, as shown, related to meromorphic functions with interdependent residues. The structure of correlations is moreover linked to the quantitative limitation of entangle-

ment between spatial regions on a fundamental level. A possible deeper significance of this formal assumption remains to be found, but similar limitations, such as the Bekenstein bound, come to mind.

One might speculate that based on the findings above—in particular the relations of higher order correlations to two- and three-point functions—some new insight into diagrammatic perturbative methods could be obtained. One future direction of investigation are virtual processes. As mentioned in the introduction, in well-known perturbative methods for interacting field theories, the states of the interacting theory are described in terms of states of the non-interacting counterpart. This leads to a description in terms of quasi-free states, which are determined by their two-point correlators, and puts the focus on propagators and an interpretation of the theory in terms of virtual processes. While this approach allows to predict experimental data with very high precision [2], it is not well understood on a fundamental level, and gives rise to conceptual problems [24]. Hence, transfer of the structures discussed in this paper to a relativistic setting might be interesting. We also note a similarity of the transforms of (continuous) MPS correlations with expressions from conformal field theory.

Of course, the relations underlying our approach are already summarized in a computationally efficient formal framework: the family of states known under the name of MPS, cMPS, and instances of PEPS. This means, given experimental data with the relations above, an optimal book-keeping device would be, *e.g.*, an MPS. However, say, series expansions in a perturbation approach starting from MPS *and potentially leaving this class of states* due to closing gaps etc. give rise to different sets of terms with different structure, and the MPS scheme is only one possible way to interpret it. A different summation order might yield a different optimal book-keeping device in this context.

In a related line of thinking, there is the possibility that the meromorphic structure of the correlations, together with the interdependencies of the poles, enable a different mathematical understanding of the underlying renormalization procedure. Such an understanding might help to find variations of the renormalization procedure, including possibly meaningful and computationally efficient extensions of MPS and cMPS to higher dimensions.

VI. ACKNOWLEDGEMENTS

We would like to thank the EU (QESSENCE), the EURYI, and the BMBF (QuORep) for support. We warmly thank Tobias J. Osborne for discussions, who emphasized that the formalism developed originally for cMPS applies equally well to MPS.

[1] M. E. Peskin and D. V. Schroeder, *An introduction to quantum field theory* (Perseus Books, 1995).
[2] R. P. Feynman, *Quantum electrodynamics* (Westview Press, 1998).
[3] G. C. Wick, Phys. Rev. **80**, 268 (1950).
[4] L. Isserlis, Biometrika **11**, 185 (1916).
[5] D. Perez-Garcia, F. Verstraete, M. M. Wolf, and J. I. Cirac, Quant. Inf. Comp. **7**, 401 (2007).
[6] M. Fannes, B. Nachtergaele, and R. F. Werner, J. Phys. A **24**, L185 (1991).
[7] J. Eisert, M. Cramer, and M. B. Plenio, Rev. Mod. Phys. **82**, 277 (2010).

[8] U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005).
[9] F. Verstraete and J. I. Cirac, Phys. Rev. Lett. **104**, 190405 (2010).
[10] T. J. Osborne, J. Eisert, and F. Verstraete, Phys. Rev. Lett. **105**, 260401 (2010).
[11] J. Haegeman, J. I. Cirac, T. J. Osborne, H. Verschelde, and F. Verstraete, Phys. Rev. Lett. **105**, 251601 (2010).
[12] N. Schuch, D. Perez-Garcia, and J. I. Cirac, Phys. Rev. B **84**, 165139 (2011).
[13] M. Sanz, M. M. Wolf, D. Perez-Garcia, and J. I. Cirac, Phys. Rev. A **79**, 042308 (2009).

- [14] M. M. Wolf, G. Ortiz, F. Verstraete, and J. I. Cirac, Phys. Rev. Lett. **97**, 110403 (2006).
- [15] S. Lloyd and S. L. Braunstein, Phys. Rev. Lett. **82**, 1784 (1999).
- [16] S. Hofferberth, I. Lesanovsky, B. Fischer, T. Schumm, and J. Schmiedmayer, Nature **449**, 324 (2007).
- [17] D. Heine, M. Wilzbach, T. Raub, B. Hessmo, and J. Schmiedmayer, Phys. Rev. A **79**, 021804 (2009).
- [18] M. M. Wolf and D. Perez-Garcia, arXiv:1005.4545.
- [19] For a discussion of the computational complexity of deciding whether or not a family of completely positive maps is generated by an underlying Markovian master equation from data taken at finitely many times, see Ref. [20].
- [20] T. S. Cubitt, J. Eisert, and M. M. Wolf, Commun. Math. Phys. **310**, 383 (2012).
- [21] M. Cramer, M. B. Plenio, S. T. Flammia, D. Gross, S. D. Bartlett, R. Somma, O. Landon-Cardinal, Y.-K. Liu, and D. Poulin, Nat. Commun. **1**, 149 (2010).
- [22] A detailed study of robustness of the scheme with respect to errors, similar to the discussion in Refs. [23], will be presented elsewhere.
- [23] S. T. Flammia, D. Gross, Y.-K. Liu, and J. Eisert, arXiv:1205.2300; M. Christandl and R. Renner, arXiv:1108.5329; R. Blume-Kohout, arXiv:1202.5270.
- [24] R. Haag, Matematisk-fysiske Meddelelser **29** (1955).

VII. APPENDIX

A. Quantum dynamical semi-groups

There is a strong formal relationship between cMPS with bond dimension d and quantum channels which are elements of a completely positive continuous one-parameter semi-group in d -dimensional Hilbert spaces, called Markovian quantum channels. For such elements T_x there exists a generator \mathcal{L} with $\mathcal{L}^*(\mathbb{1}) = 0$ such that

$$T_x = e^{x\mathcal{L}} \quad (23)$$

for all $x \geq 0$. The generator \mathcal{L} of the family of quantum channels is necessarily of the form

$$\mathcal{L}(\rho) = -i[\rho, H] - \frac{1}{2} \sum_j \left(R_j^\dagger R_j \rho + \rho R_j^\dagger R_j - 2R_j \rho R_j^\dagger \right). \quad (24)$$

Using the isomorphism relating a density matrix defined on a d -dimensional Hilbert space to its vector form in a $d \times d$ -dimensional Hilbert space,

$$\rho(x) \mapsto |\rho(x)\rangle = \sum_{i,j=1}^d \rho_{i,j}(x) |i\rangle |j\rangle, \quad (25)$$

the above generator takes the form

$$L = -iH^* \otimes \mathbb{1} + i\mathbb{1} \otimes H - \frac{1}{2} \sum_j \left(R_j^T R_j^* \otimes \mathbb{1} + \mathbb{1} \otimes R_j^\dagger R_j - 2R_j^* \otimes R_j \right). \quad (26)$$

The Liouvillians encountered above are Liouvillians in this sense, where we merely have a single Lindblad operator R . With

$$Q = iH - \frac{1}{2} R^\dagger R, \quad (27)$$

one has

$$L = Q^* \otimes \mathbb{1} + \mathbb{1} \otimes Q + R^* \otimes R, \quad (28)$$

which is Eq. (4). Since the spectrum of \mathcal{L} is taken to be non-degenerate, there exists a unique stationary state, given by

$$\rho_{ss} = \lim_{x \rightarrow \infty} e^{x\mathcal{L}}(\rho) \quad (29)$$

for every ρ . The generator is also gapped, so that convergence to the stationary state is exponential. Such families of quantum channels are sometimes referred to as being relaxing.